2-D + 1-D PEM Fuel Cell Model for the Integration in Fuel Cell System Simulations

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The aim of this work is to enable simulation-based investigation of a Proton Exchange Membrane (PEM) fuel cell system operation, with the special focus on its water management. For PEM fuel cells their multi-level interaction regarding humidity is characteristic depending on e.g. transport mechanisms, degradation and performance. In order to display these dependencies correctly, a PEM fuel cell stack model has been developed, which meets high degree of resulting details and high requirements concerning its runtime, to enable acceptable simulation times for fuel cell system simulations. The core of the model is a 2-D + 1-D structure that resolves area specific conditions, such as dry cathode inlet and wet cathode outlet conditions in dependence of principle layout variations as eg. co- or counter-flow fields. The fuel cell model as well as its possibilities with respect to the integration in system simulations is presented in this work.

KEYWORDS: FUEL CELL SYSTEM, MODELLING, SIMULATION, PEM, WATER MANAGEMENT, SYSTEM SIMULATION, CO-SIMULATION

1. INTRODUCTION

The development of fuel cell systems can be supplemented by simulation-based investigations. Those simulations need suitable models to provide stable forecasts and proper results. The developed models and simulation modules can also be used for system controlling and development by analysing their results.

The following work will propose a 2-D+1-D fuel cell stack model and its implementation into an exemplary fuel cell system to show its usability and advantages regarding the research of operation conditions and system dynamics for the development process. This paper will also show exemplary results and their importance for design studies. The simulation shown in the following allows an analysis of existing systems and the succeeding of different operation strategies and constructive influences. This work will exemplary show locally resolved and dynamical effects of a defined operation strategy and the influence of a counter-flow and co-flow of the media within the fuel cell.

2. FUEL CELL STACK

The PEM fuel cell stack model is based on a 2-D+1-D structure, which determines the species transportation through the Membrane Electrode Assembly (MEA) and is able to represent area specific conditions with a freely selectable resolution. The electrochemical calculation is based on the Kulikovsky model [Kulikovsky, 2014] and is discussed by Gößling [Gößling, 2019]. The local resolution is achieved by a

division of the flow field structure into segments of equal size. This requires a symmetric structure. The path of the cathode channel is defined to progress from segment 1 to segment n like shown in Fig. 1.

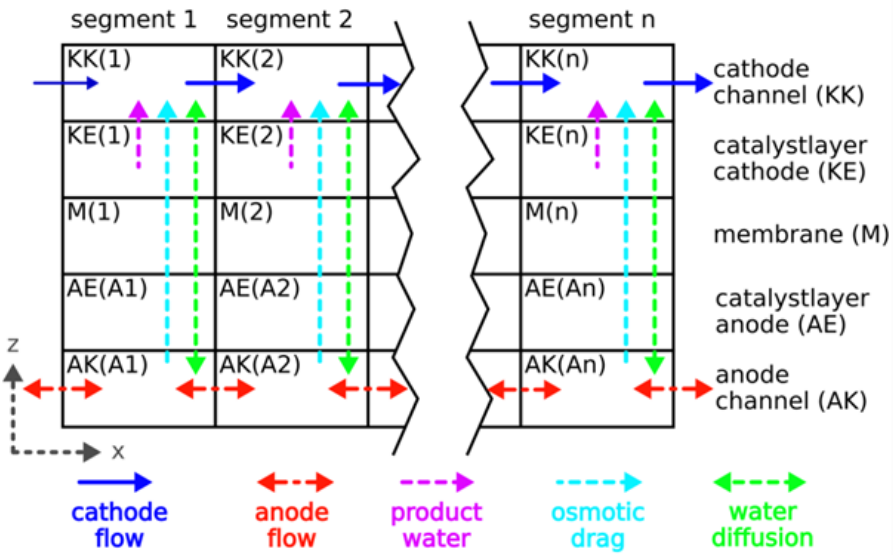

Fig. 1: 2-D + 1-D structure of the fuel cell model with segmented distribution of all layers of the MEA in relation to the cathode channel

The species transport through the MEA includes the different water transport effects and the nitrogen diffusion. The focus of the model is on the water transports, which consist of the product water generated by the electrochemical reaction, the water diffusion based on the partial pressures and the osmotic drag. This allows the investigation of locally resolved conditions such as the current density distribution and membrane humidity along the cathode and anode channel. The fuel cell stack model consists of two separately calculated 2-D+1-D models called “center cell” and “border cell” in the following. The border cell represents the two cells at the border of the stack assembly, which are close to the end plates and thus got a higher thermal mass which in turn affects the thermodynamics. The center cell is representing the remaining cells of the stack. The model is extended by a dynamical thermal model and a membrane model. The dynamical membrane model is based on the research of Satterfield and Benziger [Satterfield, 2008]. Both, the membrane and thermal model got a locally resolved resolution corresponding to the cathode.

The modelling of the fuel cell stack is realized in MATLAB/Simulink to offer a generalized and compromised solution for allocating appropriate exports for several other simulation environments. The model is fully parameterized and thus is applicable to several cell geometrics and assemblies.

3. FUEL CELL SYSTEM

The fuel cell system consists of three circuits; the anode, cathode and cooling. While cooling and anode are closed loops with the possibility to open the system

boundaries through valves, the cathode is an open circuit interacting with the ambiance. The flow chart of the fuel cell system is shown in Fig. 2.

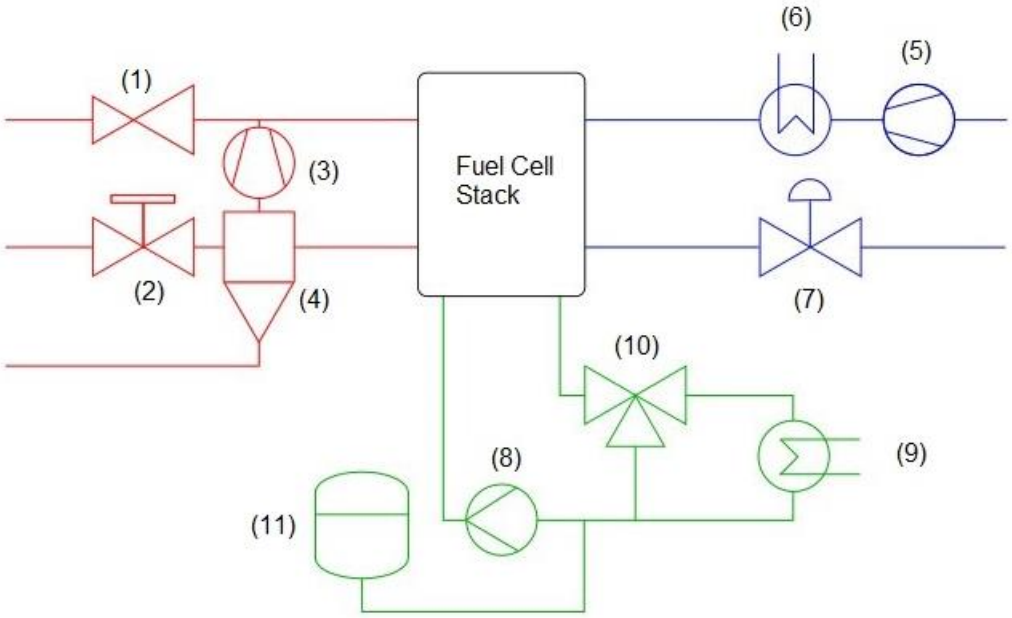

Fig. 2: Flow chart of the proposed fuel cell system including the fuel cell stack (black), the cathode circuit (blue), the anode circuit (red) and the cooling circuit (green).

The anode mass flow is supplied by a hydrogen tank and controlled on the desired outlet pressure of the fuel cell stack via a valve (1). The anode fluid then enriches throughout the reaction zone with water and nitrogen caused by diffusion from the cathode, while the hydrogen content decreases caused by the electrochemical reaction. To get rid of the undesired nitrogen another valve (2) is connected downstream, which opens at specific timings to flush (purge) the anode. This proceeding is carried out in repetitious defined intervals to keep a tolerated nitrogen ratio. The anode fluid is recirculated by a blower (3) after passing a water separator (4) separating the liquid water and then combined with the fresh hydrogen from the tank, which is replacing the consumed hydrogen by the electrochemical process.

The cathode path starts with a compressor (5) providing the air controlled on the desired stoichiometry, followed by a heat exchanger (6) by reason of the temperature increase of the compression. After passing the fuel cell stack, the air traverses a proportional valve (7) for a controlled pressurization.

The circulating mass flow of the cooling circuit is provided by a pump (8) and the heat dissipation is realized by a heat exchanger (9). The controlling of the cooling temperature is executed by a proportional valve (10). Its position is dependent of the actual and desired cooling temperature and controls the flowrate through the heat exchanger and its bypass to regulate the heat removal. Moreover, a pressure compensation tank (11) is implemented inside the cooling circuit.

The system simulation is realized in AVL Cruise M, which is a multi-disciplinary system simulation tool and can be used for concept analysis and sub-system design and virtual component integration. It also enables the usage of Hardware-in-the-Loop (HiL) environments for controlling and testing. It offers calibrateable ready-made solutions for the used system components e.g. the heat exchanger, pumps etc. The fuel stack model is exported from Simulink to make it applicable in a Co-Simulation inside AVL Cruise M.

4. CO-SIMULATION

As the stack model and the system model are realized in different software packages, a co-simulation is necessary. For realizing the co-simulation the stack model is exported from Simulink as a Functional Mock-up Unit (FMU) and implemented inside AVL Cruise M via Functional Mock-up Interface (FMI), which is a standardized interface for model exchange and co-simulations. Inside the AVL Cruise M environment the stack and system model are exchanging data via defined interfaces. AVL Cruise M treats the media flows as such with defined units while the exported fuel stack model is working with signals only. Thus the interfaces between the stack and the system are converted to be used properly. The most important

stack parameters and operation conditions used for the simulation results are summarized in Table 1.

Table 1: Parameters of the used fuel cell stack and system

Parameter	**Value**	**Unit**
Number of cells	400	-
Active area	300	cm²
Number of segments	10	-
Anode outlet pressure	2	bar abs
Cathode outlet pressure	2	bar abs
Anode stoichiometry	1.2	-
Cathode stoichiometry	2	-
Anode inlet temperature	65	°C
Cathode inlet temperature	65	°C
Coolant inlet temperature	60	°C

5. RESULTS

The results shown in the following compare two simulations with equal boundary conditions (Table 1) for the system shown in Fig. 2. One simulation has been performed with counter- and one with co-flow of the anode and cathode. The fuel cell stack is operated potentiostatic at 240 V, after passing a starting procedure. The resulting stack current over time is shown in Fig. 3. During the starting procedure the media is pre provided, to prevent an undersupply of the cathode and anode. The starting procedure takes approximately 20 seconds. Afterwards the media is controlled for a stoichiometric operation.

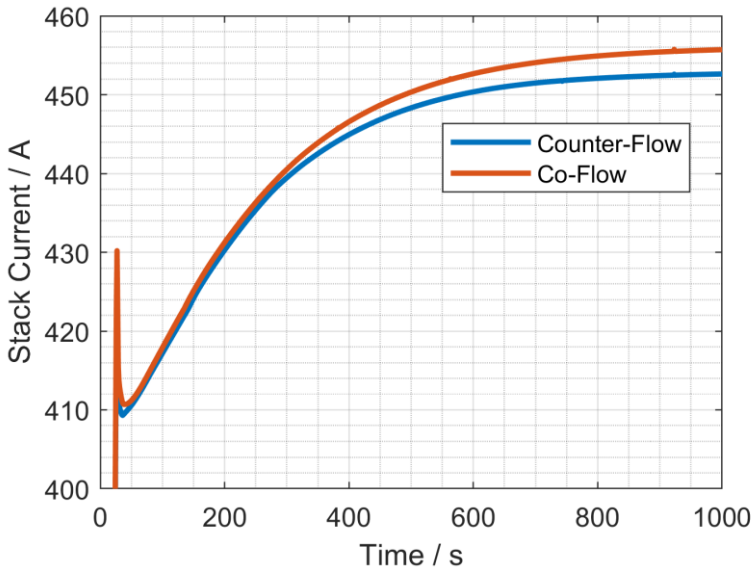

Fig. 3: Stack current over time from simulation results for counter-flow and co-flow

The stack current over time shows the influence of the dynamical start procedure. Influence factors for these dynamics are the temperatures, humidities, media transport etc. . The differences between the counter-flow and co-flow is shown exemplary by the locally resolved membrane humidity at the simulation time t = 1000 s in 4.

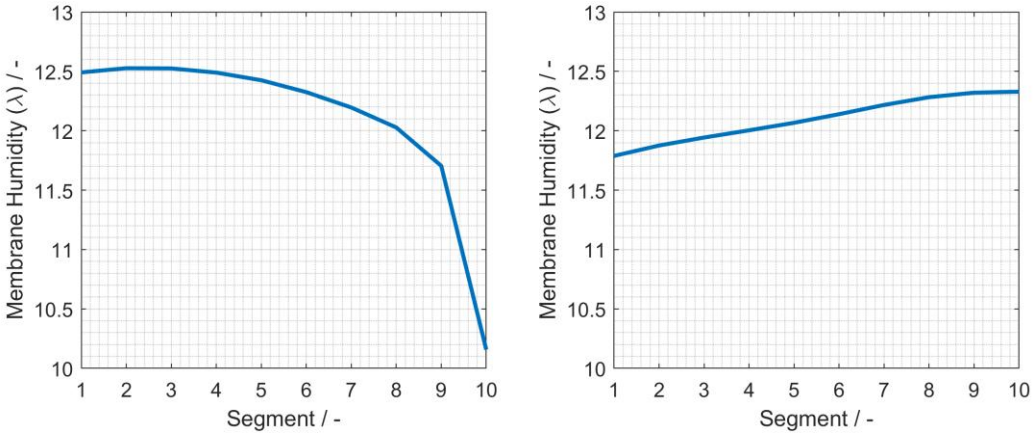

Fig. 4: Locally resolved membrane humidity for counter-flow (left) and co-flow (right)

The membrane humidity λ is defined as the ratio of the number of water molecules to the number of charge ($SO_3^- H^+$) sites [Springer, 1991]. Fig. 4 shows that the co-flow got higher membrane humidity on average with a steady increasing gradient along the cathode channel, which leads to the higher performance seen in Fig. 3. The higher membrane humidity results from the higher humidity in the anode and cathode channels. Fig. 5 shows the relative humidity at the anode inlet and outlet for both cases.

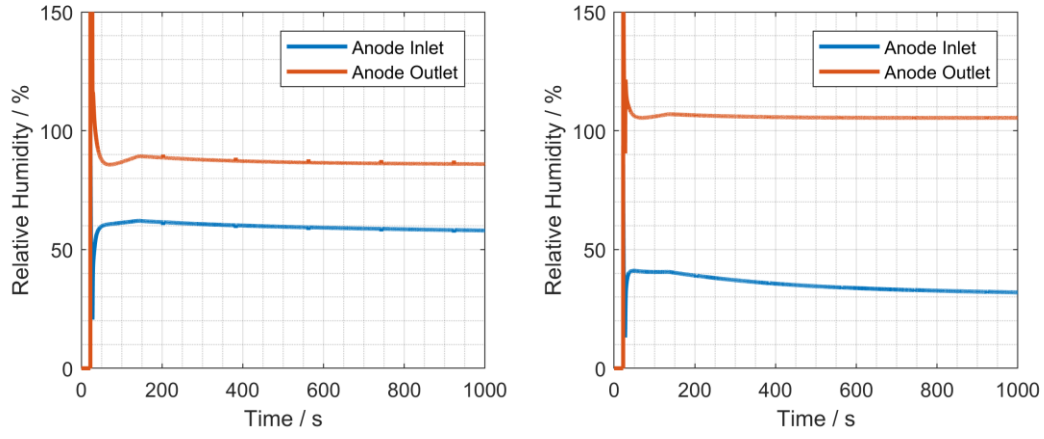

Fig. 5: Relative humidity of the anode media inlet and outlet for counter-flow (left) and co-flow (right)

The relative humidity for the co-flow at the anode outlet is above 100 %, which leads to liquid water, while for counter-flow the anode media stays gaseous except for the peak in the first seconds evoked by the high pre provision of reactant media.

6. SUMMARY

The fuel cell stack is fully parameterizable, which allows an adaption to different cell and stack assemblies and systems. The results show that dependent on the operation strategy the fuel cell stack is able to perform higher power and thus higher efficiency with a co-flow than with a counter-flow. On the other hand for the counter-flow the anode requires significantly less humidification than the co-flow for comparable power, which can be a significant advantage for system development. For different operation strategies and boundary conditions the counter-flow could lead to higher efficiency, which explains the necessity and benefits of simulating those varying strategies and parameters to optimize the fuel cell system development.

7. OUTLOOK

Further works will elaborate the optimization of the required simulation time and improve the real time capability. This real time capability enables a Hardware-in-the-Loop (HiL) simulation, which will be performed as well. Furthermore the available model will be enlarged by a degradation model based on artificial intelligence and by modelling frozen conditions and start-/stop-processes.

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